

# Comment on "Dielectric screening and plasmons in AA-stacked bilayer graphene"

Yawar Mohammadi\*

*Young Researchers and Elite Club, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran*

(Dated: October 20, 2014)

PACS numbers: 71.45.Lr, 73.22.Pr, 71.51.Gm

In reference [1], authors consider dielectric screening and plasmons in AA-stacked bilayer graphene. Some equations and results obtained in this paper seem to be incorrect. In this comment, we demonstrate this claim and present our results. At first we summarize our comments. The obtained eigenfunctions for the unbiased case, Eqs. (7) and (8), don't satisfy the Schrödinger equation. Equations (31), (32) and (33) don't satisfy the Schrödinger equation and also don't reduce to the corresponding results in the zero limit of  $V$  (the applied perpendicular electric potential). The overlap of the electron and hole wavefunctions, Eq. (35), can not be concluded from Eq. (33) and also it doesn't reduce to Eq. (17) in the zero limit of  $V$ , while it must be so. Furthermore, we show that this result for the overlap of the electron and hole wavefunctions is not correct. The main comment is that the low energy limit of the optical and acoustic plasmon dispersion relations, Eqs. (36), (37) and (39), can not be obtained by making use of Eq. (35). Plots of figure 4 can not be correct, since they have been obtained by making use of Eq. (35). Some of these mistakes arise from the used unitary transformation. For example, even if the calculations are done correctly, the biased-case eigenfunctions don't reduce to the corresponding result in the zero limit of  $V$ . In the rest of this comment we present our results.

Starting from Eq. (1) of Ref. [1] for  $\mathcal{H}$ , first we obtain a unitary transformation matrix, which can be used to transform this Hamiltonian matrix into a block-diagonalized form similar to Eq. (5) of Ref. [1] denoted, in this comment, by  $\mathcal{H}_{bd}$ . Let us suppose that  $X^\dagger \mathcal{H} X$  and  $Y^\dagger \mathcal{H}_{bd} Y$  are the transformations that diagonalize  $\mathcal{H}$  and  $\mathcal{H}_{bd}$  respectively. These matrixes,  $X$  and  $Y$ , can be written as

$$\begin{aligned} X &= \begin{pmatrix} \Phi_{+,-}(\mathbf{k}) & \Phi_{-,-}(\mathbf{k}) & \Phi_{+,+}(\mathbf{k}) & \Phi_{-,+}(\mathbf{k}) \end{pmatrix}, \\ Y &= \begin{pmatrix} \Psi_{+,-}(\mathbf{k}) & \Psi_{-,-}(\mathbf{k}) & \Psi_{+,+}(\mathbf{k}) & \Psi_{-,+}(\mathbf{k}) \end{pmatrix}, \end{aligned} \quad (1)$$

where

$$\Phi_{\lambda,s}(\mathbf{k}) = \frac{1}{2} \begin{pmatrix} 1 \\ \lambda e^{i\phi_{\mathbf{k}}} \\ -s \\ -s\lambda e^{i\phi_{\mathbf{k}}} \end{pmatrix}, \quad (2)$$

are eigenfunctions of  $\mathcal{H}$ , Eq. (1) of Ref. [1], and

$$\Psi_{\lambda,-}(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \lambda e^{i\phi_{\mathbf{k}}} \\ 0 \\ 0 \end{pmatrix}, \quad \Psi_{\lambda,+}(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ \lambda e^{i\phi_{\mathbf{k}}} \end{pmatrix}, \quad (3)$$

are eigenfunctions of  $\mathcal{H}_{bd}$ , Eq. (5) of Ref. [1], with  $s = \pm$  and  $\lambda = \pm$ . It is easy to show that these eigenfunctions satisfy the corresponding Schrödinger equations with  $\varepsilon_{\lambda,s}(\mathbf{k}) = st_1 + \lambda v_F k$ . Since  $X^\dagger \mathcal{H} X$  and  $Y^\dagger \mathcal{H}_{bd} Y$  are equal, we can conclude that  $Y X^\dagger \mathcal{H} X Y^\dagger = \mathcal{H}_{bd}$ . So we reach a unitary transformation ( $U^{-1} \mathcal{H} U = \mathcal{H}_{bd}$ ) which transforms  $\mathcal{H}$  into a block-diagonalized form as Eq. (5) of Ref. [1]. Here,  $U$  is given by

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}. \quad (4)$$

In accordance to this unitary transformation, we do  $\mathbf{V}(q) = \mathcal{U}^{-1} \tilde{\mathbf{V}}(q) \mathcal{U}$  to transform the Coulomb interaction matrix from the layer1/layer2 basis to the bonding/antibonding basis, where

$$\mathcal{U} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (5)$$

Notice that this unitary transformation leads to the same results as Eqs. (14)-(28) of Ref. [1].

Now we calculate the eigenfunctions of the Hamiltonian introduced in Eq. (29) of Ref. [1], subjected to our unitary transformation. To obtain these eigenfunctions, first we obtain the eigenfunctions of  $H_V$  denoted here by  $\psi_{\lambda,s}^V(\mathbf{k})$  and then calculate  $\Psi_{\lambda,s}^V(\mathbf{k}) = U^{-1}\psi_{\lambda,s}^V(\mathbf{k})$  which are the eigenfunctions of  $\mathcal{H}^V = U^{-1}H^V U$ . So we have

$$\Psi_{\lambda,s}^V(\mathbf{k}) = \frac{1}{2\sqrt{2t_1^V(t_1^V - sV)}} \begin{pmatrix} t_1 + (V - st_1^V) \\ (t_1 + (V - st_1^V))\lambda e^{i\phi_{\mathbf{k}}} \\ t_1 - (V - st_1^V) \\ (t_1 - (V - st_1^V))\lambda e^{i\phi_{\mathbf{k}}} \end{pmatrix}. \quad (6)$$

It is easy to show that these eigenfunctions, in zero limit of  $V$ , reduces to Eq. (3) of this comment. While if we use the unitary transformation matrix of Re. [1], the obtained eigenfunctions, in the zero limit of  $V$ , do not reproduce the correct eigenfunction introduced in Eq. (3).

By using Eq. (6) and calculating 1-loop polarization<sup>2</sup>, we obtain

$$\Pi_{s,s';\lambda,\lambda'}^V(\mathbf{q}) = -\frac{g_\sigma g_v}{L^2} \sum_{\mathbf{k}} \frac{f_{\lambda,s}(\mathbf{k}) - f_{\lambda',s'}(\mathbf{k} + \mathbf{q})}{\omega + \varepsilon_{\lambda,s}^V(\mathbf{k}) - \varepsilon_{\lambda',s'}^V(\mathbf{k} + \mathbf{q}) + i\delta} \mathcal{F}_{ss';\lambda\lambda'}^V(\mathbf{k}, \mathbf{k} + \mathbf{q}), \quad (7)$$

where  $\mathcal{F}_{ss';\lambda\lambda'}^V(\mathbf{k}, \mathbf{k}') = |\langle \Psi_{\lambda',s'}^V(\mathbf{k}') | e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}} | \Psi_{\lambda,s}^V(\mathbf{k}) \rangle|^2$  is the overlap of the electron and hole wavefunctions which is given by

$$\mathcal{F}_{ss';\lambda\lambda'}^V(\mathbf{k}, \mathbf{k} + \mathbf{q}) = \frac{1 + \lambda\lambda' \cos(\phi_{\mathbf{k}} - \phi_{\mathbf{k}+\mathbf{q}})}{2}, \quad (8)$$

if  $s = s'$  and  $\mathcal{F}_{ss';\lambda\lambda'}^V(\mathbf{k}, \mathbf{k} + \mathbf{q}) = 0$  when  $s \neq s'$ . This equation shows that the dynamical polarization of the biased AA-stacked BLG, is equal to that of doped single layer graphene with  $\mu = t_1^V$ ,  $\Pi_{SLG}^{\mu=t_1^V}(\mathbf{q}, \omega)$ . By making use of Eqs. (6) and (7), we obtain<sup>3</sup> a closed analytical expression for the real part of the polarization function as

$$\Pi^V(\mathbf{q}, \omega) = -\frac{g_\sigma g_v t_1^V}{2\pi v_F^2} + \frac{g_\sigma g_v q^2}{16\pi\sqrt{\omega^2 - v_F^2 q^2}} [G(\frac{2t_1^V + \omega}{v_F q}) - G(\frac{2t_1^V - \omega}{v_F q})], \quad (9)$$

with  $G(x) = x\sqrt{x^2 - 1} - \cosh^{-1}(x)$  while  $\text{Im}\Pi^V(\mathbf{q}, \omega) = 0$ . Notice that each cone contributes independently and their contributions are equal. This relation is valid in the region of the spectrum ( $v_F q < \omega < 2t_1^V - v_F q$ ) where it is claimed that Eq. (36) and (37) of Ref. [1] are the low energy dispersion relation for the optical and acoustic plasmon modes. It is easy to show that Eq. (36) and (37) of Ref. [1] are obtained by making use of our results, while they can not be concluded from corresponding relation in Ref. [1], Eq. (35). To demonstrate our claim, we rewrite Eq. (35) of Ref. [1] as

$$\mathcal{F}_{ss';\lambda\lambda'}^V(\mathbf{k}, \mathbf{k} + \mathbf{q}) = \frac{1 - \beta_s^2(t_1, V)}{2[1 + \beta_s^2(t_1, V)]} + \frac{\beta_s^2(t_1, V)}{1 + \beta_s^2(t_1, V)} \frac{1 + \lambda\lambda' \cos(\phi_{\mathbf{k}} - \phi_{\mathbf{k}+\mathbf{q}})}{2}, \quad (10)$$

for  $s = s'$ . So we can obtain an analytical relation for the real part of the dynamical polarization function as

$$\Pi^V(\mathbf{q}, \omega) = \frac{\beta_s^2(t_1, V)}{1 + \beta_s^2(t_1, V)} \Pi_{SLG}^{\mu=t_1^V}(\mathbf{q}, \omega) + \frac{1 - \beta_s^2(t_1, V)}{[1 + \beta_s^2(t_1, V)]} \Pi'(\mathbf{q}, \omega), \quad (11)$$

being valid in the region  $v_F q < \omega < 2t_1^V - v_F q$ , where

$$\Pi'(\mathbf{q}, \omega) = \frac{g_\sigma g_v q^2}{16\pi\sqrt{\omega^2 - v_F^2 q^2}} [G(\frac{2t_1^V + \omega}{v_F q}) - G(\frac{2t_1^V - \omega}{v_F q})] - \frac{g_\sigma g_v q^2 \sqrt{\omega^2 - v_F^2 q^2}}{16\pi} [\cosh^{-1}(\frac{2t_1^V + \omega}{v_F q}) - \cosh^{-1}(\frac{2t_1^V - \omega}{v_F q})] \quad (12)$$

One can show easily that Eqs. (36) and (37) of Ref. [1] can not be concluded from Eqs. 11 and 12 of this comment obtained from Eq. (35) of Ref. [1].

In summary, we showed that some equations obtained in Ref. [1] are not correct. Furthermore, we present our results which seems to be correct.

## References

---

\* yawar.mohammadi@gmail.com

<sup>1</sup> R. Roldan, L. Brey, Phys. Rev. B **88**, 115420 (2013).

<sup>2</sup> Y. Mohammadi, R. Moradian and F. Sirzadi Tabar, Solid State Commun. **193**, 1 (2014).

<sup>3</sup> B. Wunsch, T. Stauber, F. Sols, F. Guinea, New. J. Phys. **8**, 318 (2006).